



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:34 am BST

PDB ID : 1E02  
Title : Porcine Odorant Binding Protein Complexed with undecanal  
Authors : Vincent, F.; Spinelli, S.; Cambillau, C.; Tegoni, M.  
Deposited on : 2000-03-09  
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

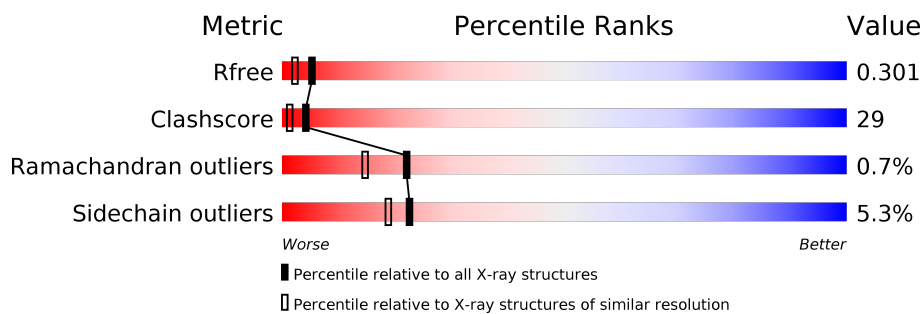
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	157	
1	B	157	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNA	A	600	-	-	X	-
2	UNA	B	600	-	-	X	-

## 2 Entry composition [i](#)

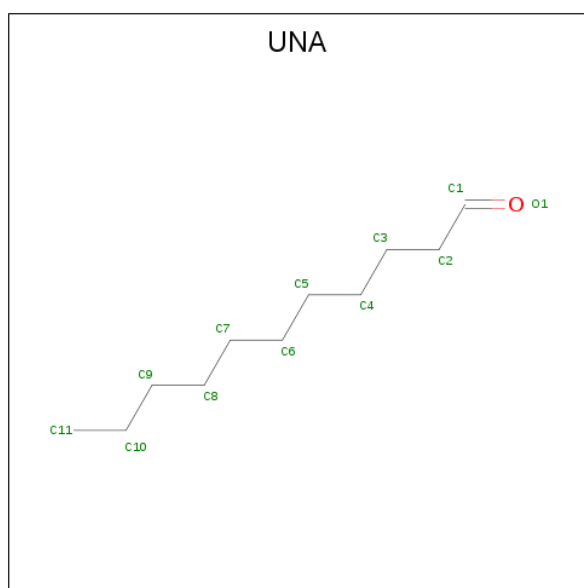
There are 3 unique types of molecules in this entry. The entry contains 2573 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ODORANT-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	149	1186	745	185	250	6	16	3	0
1	B	147	1161	727	183	247	4	29	0	0

- Molecule 2 is UNDECANAL (three-letter code: UNA) (formula:  $C_{11}H_{22}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	11	1	0	0
2	B	1	12	11	1	0	0

- Molecule 3 is water.

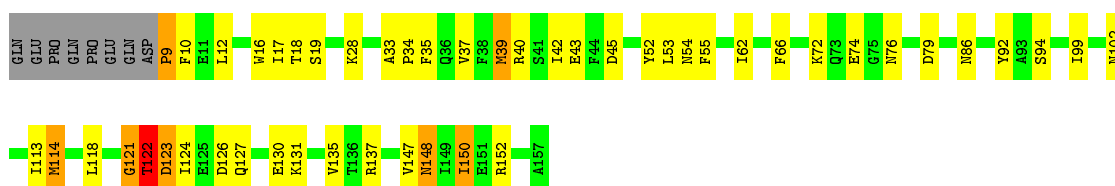
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	114	Total 114	O 114	0	0
3	B	88	Total 88	O 88	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

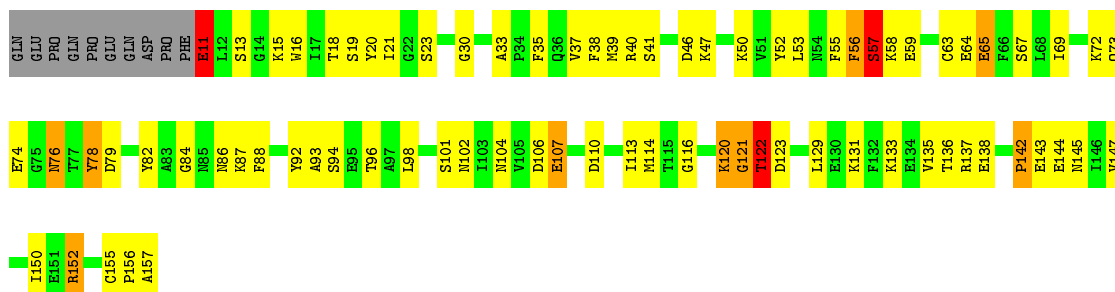
- Molecule 1: ODORANT-BINDING PROTEIN

Chain A: 



- Molecule 1: ODORANT-BINDING PROTEIN

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.78Å 87.91Å 92.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.15 17.93 – 2.15	Depositor EDS
% Data completeness (in resolution range)	90.7 (18.00-2.15) 90.8 (17.93-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.35 (at 2.15Å)	Xtrriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.192 , 0.256 0.243 , 0.301	Depositor DCC
$R_{free}$ test set	828 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtrriage
Anisotropy	0.008	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.032 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: UNA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.63	2/1220 (0.2%)	0.79	5/1641 (0.3%)
1	B	2.40	63/1178 (5.3%)	1.32	6/1586 (0.4%)
All	All	1.74	65/2398 (2.7%)	1.08	11/3227 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	GLY	C-N	-15.03	0.99	1.34
1	B	16	TRP	CD2-CE2	-9.96	1.29	1.41
1	B	107	GLU	CD-OE2	9.74	1.36	1.25
1	B	65	GLU	CG-CD	-9.63	1.37	1.51
1	B	92	TYR	CG-CD1	9.32	1.51	1.39
1	B	143	GLU	N-CA	-9.21	1.27	1.46
1	B	41	SER	CB-OG	-9.14	1.30	1.42
1	B	142	PRO	N-CD	8.46	1.59	1.47
1	B	116	GLY	C-O	-8.12	1.10	1.23
1	B	121	GLY	C-N	-8.10	1.15	1.34
1	B	64	GLU	C-O	8.00	1.38	1.23
1	B	64	GLU	CD-OE1	-7.79	1.17	1.25
1	B	84	GLY	C-O	-7.79	1.11	1.23
1	B	94	SER	CB-OG	7.60	1.52	1.42
1	B	64	GLU	CD-OE2	7.58	1.33	1.25
1	B	82	TYR	CD2-CE2	-7.58	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	SER	CA-CB	-7.56	1.41	1.52
1	B	40	ARG	CZ-NH2	-7.56	1.23	1.33
1	B	20	TYR	N-CA	-7.47	1.31	1.46
1	B	74	GLU	CD-OE1	7.17	1.33	1.25
1	B	67	SER	CB-OG	-7.01	1.33	1.42
1	B	143	GLU	CG-CD	6.96	1.62	1.51
1	B	107	GLU	CB-CG	-6.72	1.39	1.52
1	B	78	TYR	CE1-CZ	6.62	1.47	1.38
1	B	113	ILE	C-O	-6.57	1.10	1.23
1	B	106	ASP	CB-CG	6.57	1.65	1.51
1	B	11	GLU	C-N	-6.43	1.19	1.34
1	B	136	THR	CB-OG1	-6.35	1.30	1.43
1	B	82	TYR	CB-CG	6.20	1.60	1.51
1	B	155	CYS	CB-SG	-6.17	1.71	1.82
1	B	145	ASN	C-O	-6.17	1.11	1.23
1	B	98	LEU	C-O	-6.11	1.11	1.23
1	B	59	GLU	CD-OE2	-6.04	1.19	1.25
1	B	20	TYR	C-O	-6.02	1.11	1.23
1	B	56	PHE	CE2-CZ	6.01	1.48	1.37
1	B	138	GLU	N-CA	5.97	1.58	1.46
1	B	38	PHE	CG-CD2	-5.95	1.29	1.38
1	B	52	TYR	CB-CG	5.95	1.60	1.51
1	B	144	GLU	CD-OE1	-5.94	1.19	1.25
1	B	122	THR	C-N	-5.92	1.20	1.34
1	B	23	SER	CA-CB	-5.90	1.44	1.52
1	B	96	THR	CB-OG1	-5.86	1.31	1.43
1	B	79	ASP	C-N	-5.78	1.20	1.34
1	B	56	PHE	CB-CG	-5.73	1.41	1.51
1	B	78	TYR	CG-CD1	5.73	1.46	1.39
1	B	120	LYS	C-N	-5.72	1.22	1.33
1	B	47	LYS	N-CA	5.71	1.57	1.46
1	B	137	ARG	CA-C	-5.67	1.38	1.52
1	B	15	LYS	CA-CB	-5.60	1.41	1.53
1	B	93	ALA	C-O	-5.56	1.12	1.23
1	B	137	ARG	C-O	5.56	1.33	1.23
1	B	78	TYR	C-O	-5.49	1.12	1.23
1	B	147	VAL	CA-C	-5.47	1.38	1.52
1	B	82	TYR	CZ-OH	5.45	1.47	1.37
1	B	155	CYS	N-CA	5.44	1.57	1.46
1	B	147	VAL	C-N	-5.37	1.21	1.34
1	B	57	SER	CB-OG	-5.35	1.35	1.42
1	B	21	ILE	C-O	-5.34	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	16	TRP	CE3-CZ3	-5.28	1.29	1.38
1	B	142	PRO	CA-C	5.25	1.63	1.52
1	B	67	SER	CA-CB	-5.22	1.45	1.52
1	B	101	SER	CB-OG	-5.07	1.35	1.42
1	A	9	PRO	N-CD	5.06	1.54	1.47
1	B	37	VAL	CB-CG2	-5.06	1.42	1.52
1	B	59	GLU	CD-OE1	-5.04	1.20	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	GLY	C-N-CA	9.31	144.97	121.70
1	B	122	THR	O-C-N	8.75	136.70	122.70
1	A	122	THR	O-C-N	8.03	135.55	122.70
1	B	122	THR	CA-C-N	-7.46	100.78	117.20
1	A	123	ASP	N-CA-CB	-6.62	98.69	110.60
1	B	20	TYR	O-C-N	-6.47	112.34	122.70
1	A	122	THR	CA-C-N	-6.24	103.47	117.20
1	A	39[A]	MET	CG-SD-CE	5.83	109.53	100.20
1	A	39[B]	MET	CG-SD-CE	5.83	109.53	100.20
1	B	53	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	106	ASP	CB-CG-OD1	5.21	122.99	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	LYS	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1186	0	1132	73	0
1	B	1161	0	1102	52	0
2	A	12	0	22	33	0
2	B	12	0	22	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	114	0	0	3	0
3	B	88	0	0	15	0
All	All	2573	0	2278	134	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39[B]:MET:CE	2:A:600:UNA:H62	1.32	1.52
1:B:122:THR:CG2	1:B:123:ASP:N	1.81	1.30
1:B:122:THR:HG23	1:B:123:ASP:CA	1.66	1.25
1:A:39[B]:MET:CE	2:A:600:UNA:C6	2.28	1.11
1:A:122:THR:CG2	1:A:123:ASP:N	2.05	1.11
1:B:122:THR:HG23	1:B:123:ASP:CB	1.82	1.09
1:A:72:LYS:HE2	3:A:2051:HOH:O	1.51	1.08
1:A:122:THR:HG23	1:A:123:ASP:N	1.52	1.07
1:A:39[B]:MET:HE2	2:A:600:UNA:H62	1.33	1.07
1:A:39[B]:MET:CG	2:A:600:UNA:H72	1.83	1.06
1:A:39[B]:MET:HG3	2:A:600:UNA:H72	1.36	1.06
1:A:39[B]:MET:HE1	2:A:600:UNA:H62	1.07	1.05
2:B:600:UNA:H61	2:B:600:UNA:O1	1.58	1.02
2:B:600:UNA:C1	2:B:600:UNA:H91	1.90	1.01
1:B:110:ASP:O	3:B:2060:HOH:O	1.84	0.94
1:A:39[B]:MET:HE1	2:A:600:UNA:C6	1.92	0.94
1:B:122:THR:HG23	1:B:123:ASP:N	1.19	0.91
1:A:12:LEU:HD21	3:B:2018:HOH:O	1.70	0.90
1:A:122:THR:HG23	1:A:123:ASP:CA	2.02	0.88
1:A:39[B]:MET:HE1	2:A:600:UNA:H42	1.56	0.88
1:A:122:THR:HG23	1:A:123:ASP:CB	2.04	0.86
1:B:157:ALA:HB2	3:B:2088:HOH:O	1.76	0.86
1:A:39[B]:MET:SD	2:A:600:UNA:H62	2.16	0.85
1:A:39[A]:MET:HE1	1:A:55:PHE:HB3	1.57	0.85
2:B:600:UNA:C1	2:B:600:UNA:H61	2.06	0.84
1:A:39[A]:MET:HE3	2:A:600:UNA:H42	1.59	0.84
1:A:53:LEU:HD22	2:A:600:UNA:H41	1.59	0.83
1:A:39[B]:MET:HE1	2:A:600:UNA:C4	2.13	0.78
1:A:39[A]:MET:CG	2:A:600:UNA:H72	2.12	0.77
1:B:55:PHE:CZ	2:B:600:UNA:H113	2.19	0.77
1:B:55:PHE:CE2	2:B:600:UNA:C11	2.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39[A]:MET:HG2	2:A:600:UNA:H72	1.66	0.76
1:B:122:THR:CG2	1:B:123:ASP:CB	2.63	0.75
1:A:39[A]:MET:CE	1:A:55:PHE:HB3	2.20	0.72
1:A:39[B]:MET:CE	2:A:600:UNA:H42	2.20	0.71
1:B:55:PHE:CE2	2:B:600:UNA:H112	2.27	0.70
1:A:122:THR:CG2	1:A:123:ASP:O	2.40	0.69
1:B:157:ALA:CB	3:B:2088:HOH:O	2.34	0.68
1:A:39[B]:MET:SD	2:A:600:UNA:C6	2.80	0.68
1:A:10:PHE:HE2	1:A:94:SER:HA	1.59	0.67
2:B:600:UNA:O1	2:B:600:UNA:H91	1.95	0.67
1:A:39[B]:MET:SD	2:A:600:UNA:H72	2.33	0.67
1:A:39[B]:MET:SD	2:A:600:UNA:H42	2.35	0.66
1:A:122:THR:HG23	1:A:123:ASP:HB3	1.77	0.66
1:B:55:PHE:CZ	2:B:600:UNA:C11	2.78	0.65
1:A:122:THR:HG22	1:A:123:ASP:O	1.96	0.65
1:B:69:ILE:HG13	3:B:2041:HOH:O	1.95	0.65
1:A:86:ASN:HB3	1:A:102:ASN:HD21	1.60	0.64
1:A:53:LEU:HD13	2:A:600:UNA:C3	2.27	0.64
1:B:46:ASP:HB3	3:B:2023:HOH:O	1.98	0.64
2:B:600:UNA:C1	2:B:600:UNA:C9	2.71	0.64
1:A:39[B]:MET:SD	2:A:600:UNA:C7	2.87	0.63
1:B:122:THR:HG23	1:B:123:ASP:HB2	1.78	0.62
1:A:39[A]:MET:CE	2:A:600:UNA:H42	2.30	0.62
1:A:39[A]:MET:HG3	2:A:600:UNA:H72	1.81	0.61
1:B:122:THR:CG2	1:B:123:ASP:HB2	2.32	0.60
1:A:39[B]:MET:HE2	2:A:600:UNA:C6	2.12	0.59
1:A:53:LEU:HD13	2:A:600:UNA:H31	1.85	0.59
1:A:19[B]:SER:HB3	1:A:124:ILE:HD11	1.86	0.58
1:A:43:GLU:HB2	1:A:52:TYR:HB2	1.86	0.58
1:B:122:THR:HG23	1:B:123:ASP:CG	2.25	0.56
1:A:131:LYS:O	1:A:135:VAL:HG23	2.05	0.56
1:A:147:VAL:CG2	1:A:152:ARG:HE	2.20	0.55
1:A:53:LEU:HD13	2:A:600:UNA:H41	1.89	0.55
2:B:600:UNA:C9	2:B:600:UNA:H1	2.37	0.54
1:B:86:ASN:HD22	1:B:102:ASN:HD21	1.54	0.54
1:A:39[A]:MET:SD	2:A:600:UNA:H62	2.48	0.54
1:A:37:VAL:HG13	1:A:55:PHE:CD2	2.43	0.53
1:B:56:PHE:CZ	1:B:156:PRO:HG2	2.42	0.53
2:B:600:UNA:C6	2:B:600:UNA:O1	2.47	0.52
2:B:600:UNA:H1	2:B:600:UNA:H91	1.85	0.51
1:B:11:GLU:C	1:B:13:SER:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LYS:HE2	3:B:2014:HOH:O	2.13	0.48
1:B:72:LYS:HG2	1:B:78:TYR:CE2	2.47	0.48
1:B:152:ARG:NH1	3:B:2084:HOH:O	2.38	0.48
1:B:102:ASN:CB	2:B:600:UNA:H51	2.43	0.48
1:A:118:LEU:HD21	2:A:600:UNA:H71	1.95	0.48
1:A:53:LEU:HD13	2:A:600:UNA:C4	2.44	0.47
1:A:53:LEU:CD2	2:A:600:UNA:H41	2.38	0.47
1:B:76:ASN:ND2	3:B:2045:HOH:O	2.47	0.47
1:B:35:PHE:CD2	1:B:114:MET:SD	3.08	0.46
1:B:142:PRO:CD	3:B:2008:HOH:O	2.63	0.46
1:A:148:ASN:HD22	1:A:148:ASN:C	2.18	0.46
1:A:102:ASN:HB3	1:A:114[B]:MET:HG3	1.98	0.45
1:B:122:THR:CG2	1:B:123:ASP:CG	2.83	0.45
1:A:114[A]:MET:HE2	1:A:114[A]:MET:HB2	1.79	0.45
1:A:150:ILE:HG13	1:A:150:ILE:H	1.52	0.45
1:B:131:LYS:O	1:B:135:VAL:HG23	2.17	0.45
1:B:35:PHE:CD2	2:B:600:UNA:H41	2.52	0.45
1:A:127:GLN:NE2	3:A:2091:HOH:O	2.45	0.45
1:A:33:ALA:HB1	1:A:34:PRO:HD2	2.00	0.44
1:B:86:ASN:ND2	1:B:102:ASN:HD21	2.15	0.44
2:A:600:UNA:H111	2:A:600:UNA:H82	1.79	0.44
1:B:35:PHE:HD2	2:B:600:UNA:H41	1.81	0.44
1:A:126:ASP:O	1:A:130:GLU:HG2	2.17	0.44
2:A:600:UNA:H51	2:A:600:UNA:H82	1.68	0.44
1:A:45:ASP:HB2	1:A:52:TYR:HE2	1.83	0.43
1:B:57:SER:HB3	3:B:2031:HOH:O	2.18	0.43
1:B:39:MET:HA	1:B:55:PHE:HB3	2.01	0.43
1:A:17:ILE:HG13	1:A:121:GLY:HA2	1.99	0.43
1:B:58:LYS:HE2	1:B:63:CYS:SG	2.59	0.43
1:A:28:LYS:O	1:A:35:PHE:HB2	2.18	0.43
1:A:18:THR:OG1	1:A:39[B]:MET:HG2	2.18	0.43
1:A:39[B]:MET:HG3	2:A:600:UNA:C7	2.27	0.43
1:A:54:ASN:HA	1:A:66:PHE:O	2.19	0.43
1:A:39[B]:MET:HE2	1:A:42:ILE:HD11	2.00	0.42
1:B:86:ASN:HD21	1:B:104:ASN:HD22	1.67	0.42
1:B:107:GLU:HG3	3:B:2059:HOH:O	2.18	0.42
1:B:35:PHE:HZ	1:B:86:ASN:HD21	1.67	0.42
1:B:87:LYS:HD3	3:B:2043:HOH:O	2.20	0.42
1:B:39:MET:HE1	1:B:55:PHE:HD2	1.85	0.42
1:B:30:GLY:O	1:B:33:ALA:HB3	2.20	0.42
1:B:18:THR:O	1:B:150:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:PHE:CE1	1:B:65:GLU:HB2	2.55	0.42
1:A:118:LEU:HD21	2:A:600:UNA:C7	2.50	0.41
1:A:39[A]:MET:CE	1:A:55:PHE:CD1	3.03	0.41
1:B:122:THR:CG2	1:B:123:ASP:CA	2.61	0.41
1:A:40:ARG:HA	1:A:40:ARG:HD3	1.92	0.41
1:B:104:ASN:HB2	1:B:114:MET:HE1	2.03	0.41
1:A:137:ARG:NH1	1:B:107:GLU:HG2	2.36	0.41
1:A:16:TRP:O	1:A:39[A]:MET:HB3	2.20	0.41
1:A:42:ILE:HG23	1:A:53:LEU:HD23	2.02	0.41
1:A:102:ASN:O	1:A:113:ILE:HD12	2.21	0.41
1:B:129:LEU:HD22	1:B:133:LYS:HE3	2.03	0.41
1:B:142:PRO:HD3	3:B:2008:HOH:O	2.21	0.40
1:B:19:SER:HA	1:B:150:ILE:HG23	2.03	0.40
1:B:88:PHE:HB3	1:B:102:ASN:OD1	2.20	0.40
1:B:133:LYS:NZ	3:B:2070:HOH:O	2.52	0.40
1:B:152:ARG:HD2	1:B:152:ARG:H	1.85	0.40
1:A:102:ASN:HB3	1:A:114[B]:MET:CG	2.51	0.40
1:A:35:PHE:CD1	1:A:114[A]:MET:HE1	2.57	0.40
1:A:92:TYR:HB3	1:A:99:ILE:HB	2.03	0.40
1:A:9:PRO:N	3:A:2001:HOH:O	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	150/157 (96%)	145 (97%)	5 (3%)	0	100 100
1	B	145/157 (92%)	129 (89%)	14 (10%)	2 (1%)	11 5
All	All	295/314 (94%)	274 (93%)	19 (6%)	2 (1%)	22 15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	THR
1	B	121	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/140 (96%)	126 (93%)	9 (7%)	16	11
1	B	130/140 (93%)	124 (95%)	6 (5%)	27	23
All	All	265/280 (95%)	250 (94%)	15 (6%)	22	16

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	74	GLU
1	A	76	ASN
1	A	79	ASP
1	A	114[A]	MET
1	A	114[B]	MET
1	A	122	THR
1	A	148	ASN
1	A	150	ILE
1	B	11	GLU
1	B	57	SER
1	B	73	GLN
1	B	76	ASN
1	B	122	THR
1	B	152	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	85	ASN

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Mol	Chain	Res	Type
1	A	145	ASN
1	A	148	ASN
1	B	73	GLN
1	B	85	ASN
1	B	86	ASN
1	B	145	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	UNA	A	600	-	11,11,11	1.16	2 (18%)	10,10,10	1.39	1 (10%)
2	UNA	B	600	-	11,11,11	1.74	1 (9%)	10,10,10	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UNA	A	600	-	-	7/8/9/9	-
2	UNA	B	600	-	-	7/8/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	UNA	O1-C1	5.23	1.49	1.19
2	A	600	UNA	C7-C8	2.35	1.64	1.51
2	A	600	UNA	C3-C2	2.26	1.61	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	UNA	O1-C1-C2	-3.72	102.48	126.89

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	UNA	C6-C7-C8-C9
2	A	600	UNA	C5-C6-C7-C8
2	A	600	UNA	C11-C10-C9-C8
2	B	600	UNA	C7-C8-C9-C10
2	B	600	UNA	C2-C3-C4-C5
2	A	600	UNA	C4-C5-C6-C7
2	B	600	UNA	C4-C5-C6-C7
2	A	600	UNA	C2-C3-C4-C5
2	A	600	UNA	C6-C7-C8-C9
2	B	600	UNA	C5-C6-C7-C8
2	A	600	UNA	C3-C4-C5-C6
2	B	600	UNA	C11-C10-C9-C8
2	B	600	UNA	C1-C2-C3-C4
2	A	600	UNA	C7-C8-C9-C10

There are no ring outliers.

2 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	UNA	33	0
2	B	600	UNA	15	0



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	122:THR	C	123:ASP	N	1.20
1	B	11:GLU	C	12:LEU	N	1.19
1	B	121:GLY	C	122:THR	N	1.15
1	A	121:GLY	C	122:THR	N	0.99

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.